

chain nodes :

19 20 21 24 29 31 38 39 45

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

2-24 5-29 9-31 12-38 14-39 17-45 19-20 20-21 21-24 29-31 38-39

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18

exact/norm bonds :

1-2 1-6 2-3 2-24 3-4 4-5 5-6 5-29 7-8 7-12 8-9 9-10 9-31 10-11 11-12 12-38
14-39 17-45 19-20 20-21 21-24 29-31 38-39

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18

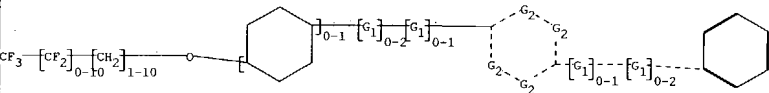
G1:C,O

G2:C,O,N

G3:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 24:CLASS 29:CLASS 31:CLASS 38:CLASS 39:CLASS 45:CLASS



chain nodes :
19 20 21 24 29 31 38 39
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
2-24 5-29 9-31 12-38 14-39 19-20 20-21 21-24 29-31 38-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18
exact/norm bonds :
1-2 1-6 2-3 2-24 3-4 4-5 5-6 5-29 7-8 7-12 8-9 9-10 9-31 10-11 11-12 12-38
14-39 19-20 20-21 21-24 29-31 38-39
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

G1:C,O
G2:C,O,N
G3:C,O
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 24:CLASS 29:CLASS 31:CLASS 38:CLASS 39:CLASS

Ring System Data

Absolute stereochemistry.



PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	557.8+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	83.97+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.4+/-45.0 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	20		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	pH 8	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	11.60	pH 1	(1) ACD
logD (LOGD)	11.60	pH 4	(1) ACD
logD (LOGD)	11.60	pH 7	(1) ACD
logD (LOGD)	11.60	pH 8	(1) ACD
logD (LOGD)	11.60	pH 10	(1) ACD
logP (LOGP)	11.598+/-0.889		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	644.61		(1) ACD
Vapor Pressure (VP)	1.78E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

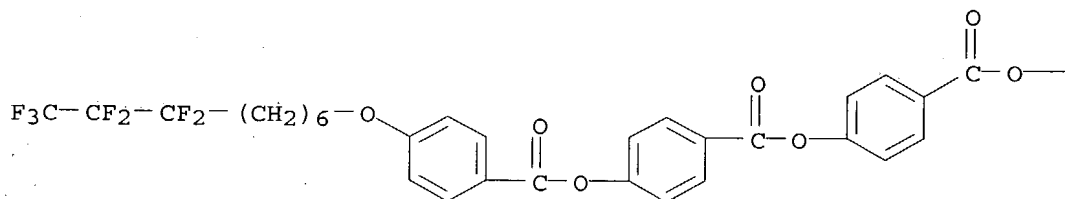
See HELP PROPERTIES for information about property data sources in REGISTRY.

L3 ANSWER 522 OF 682 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 212779-64-1 REGISTRY
 ED Entered STN: 15 Oct 1998
 CN Benzoic acid, 4-[[4-[(7,7,8,8,9,9,9-heptafluorononyl)oxy]benzoyl]oxy]-,
 4-[[[(1-methylheptyl)oxy]carbonyl]phenyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C38 H41 F7 O7
 SR CA
 LC STN Files: CA, CAPLUS

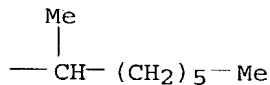
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	3

PAGE 1-A



PAGE 1-B



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD

Boiling Point (BP)	697.1+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	102.09+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	361.2+/-47.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	23		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	pH 8	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	12.61	pH 1	(1) ACD
logD (LOGD)	12.61	pH 4	(1) ACD
logD (LOGD)	12.61	pH 7	(1) ACD
logD (LOGD)	12.61	pH 8	(1) ACD
logD (LOGD)	12.61	pH 10	(1) ACD
logP (LOGP)	12.605+/-0.872		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	742.72		(1) ACD
Vapor Pressure (VP)	2.78E-19 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 131:163647 CA
TI Synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases
AU Nguyen, H. T.; Rouillon, J. C.; Babeau, A.; Marcerou, J. P.; Sigaud, G.; Cotrait, M.; Allouchi, H.
CS Centre de Recherche Paul Pascal, Universite de Bordeaux I, Pessac, 33600, Fr.
SO Liquid Crystals (1999), 26(7), 1007-1019
CODEN: LICRE6; ISSN: 0267-8292
PB Taylor & Francis Ltd.
DT Journal
LA English
CC 75-11 (Crystallography and Liquid Crystals)
Section cross-reference(s): 25, 74, 76
AB A new chiral and semiperfluorinated series with ferro and anticlinic properties was synthesized and characterized. The mesomorphic behavior was established on the grounds of both microscopic observations and DSC measurements. The nonchiral intermediate Et 4-semiperfluorinated alkyloxybenzoates exhibit SmA phases, unusual for compds. with a single Ph ring. The final derivs. display SmA, SmC* and in several cases SmCA* phases. The longer fluorinated chains favor the SmA and SmC* phases at the expense of the SmCA* phase. Electrooptical measurements were carried out with the classical SSFLC geometry. The spontaneous polarization and tilt angle at saturation are higher than those of the hydrogenous homologs, around 140 nC cm⁻² at 40°. One compound of the series the 4,4,5,5,6,6,7,7,8,8,8-nonafluoroheptyloxy derivative crystallizes in the triclinic system, space group P1, with Z = 1 (4 mols./Z). The mols. are arranged in a head-to-tail fashion with two mols. oriented in the same direction and the two others in the opposite direction. They give rise to

- sheets with a smectic C-like arrangement. The final reliability factors were $R = 0.117$ and $WR = 0.134$; the goodness of fit was $S = 1.366$.
- ST methylheptyl fluorinated alkoxybenzoyloxybenzoyloxybenzoate prepn smectic liq crystal; mol structure methylheptyl fluoroheptyloxybenzoyloxybenzoyloxybenzoate; crystal structure methylheptyl fluoroheptyloxybenzoyloxybenzoyloxybenzoate
- IT Liquid crystals
(antiferroelec.; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)
- IT Liquid crystals
(ferroelec.; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)
- IT Antiferroelectric materials
Ferroelectric materials
(liquid-crystal; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)
- IT Crystal structure
Molecular structure
(of methylheptyl nonafluoroheptyloxybenzoyloxybenzoyloxybenzoate)
- IT Electrooptical effect
Phase transition enthalpy
(of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoate liquid crystals)
- IT Liquid crystals
(smectic A; preparation and properties of Et semiperfluorinated alkyloxybenzoates and methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoates)
- IT Liquid crystals
(smectic; preparation and phase behavior of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoates)
- IT Ferroelectricity
(spontaneous polarization; of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoate liquid crystals)
- IT 237754-96-0P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and crystal structure and liquid-crystal properties of)
- IT 212779-64-1P 237754-87-9P 237754-88-0P 237754-89-1P 237754-90-4P
237754-91-5P 237754-92-6P 237754-93-7P 237754-94-8P 237754-95-9P
237754-97-1P 237754-98-2P 237754-99-3P 237755-01-0P 237755-03-2P
237755-04-3P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and liquid crystal properties of)
- IT 212779-66-3P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and liquid-crystal and electrooptic properties of)
- RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
- (1) Anon; International Tables for X-Ray Crystallography 1974, VIV
 - (2) Bennett, G; J chem Soc 1939, P420 CAPLUS
 - (3) Chandani, A; Jpn J appl Phys 1989, V28, P1261
 - (4) Doi, T; J mater Chem 1991, V1, P169 CAPLUS
 - (5) Drzewinski, W; Proceedings of the 6th International Conference on FLCs 1997, P156
 - (6) Faye, V; Liq Cryst 1995, V19, P47 CAPLUS
 - (7) Goodby, J; Nature 1989, V337, P449 CAPLUS
 - (8) Ivashenko, A; Mol Cryst liq Cryst 1981, V67, P235
 - (9) Janulis, E; Ferroelectrics 1988, V85, P375
 - (10) Kromm, P; Acta Cryst 1995, VC51, P1229 CAPLUS
 - (11) Kromm, P; Liq Cryst 1996, V21, P121 CAPLUS

- (12) Kromm, P; Liq Cryst 1996, V21, P95 CAPLUS
- (13) Kromm, P; Mol Cryst liq Cryst 1994, V257, P9 CAPLUS
- (14) Liu, H; Liq Cryst 1996, V20, P581 CAPLUS
- (15) Liu, H; Liq Cryst 1997, V22, P217 CAPLUS
- (16) Lose, D; Liq Cryst 1998, V24, P707 CAPLUS
- (17) Matsunaga, Y; Mol Cryst liq Cryst 1986, V141, P321 CAPLUS
- (18) Nguyen, H; Liq Cryst 1991, V10, P389
- (19) North, A; Acta Cryst 1968, VA24, P351
- (20) Pucci, D; Liq Cryst 1996, V21, P153 CAPLUS
- (21) Sheldrick, G; Shelxs86 Program for the Solution of Crystal Structures 1986
- (22) Sheldrick, G; Shelxs93 Program for the Refinement of Crystal Structures 1993
- (23) Takenaka, S; J chem Soc chem Commun 1992, P1748 CAPLUS
- (24) Tournilhac, F; Ferroelectrics 1991, V114, P283 CAPLUS
- (25) Twieg, R; SPIE 1991, V1455, P86

REFERENCE 2

- AN 129:237922 CA
- TI Dielectric, optical and TSM measurements on semi-perfluoro ferro- and antiferroelectric liquid crystals
- AU Sarmento, S.; Carvalho, P. Simeao; Glogarova, M.; Chaves, M. R.; Nguyen, H. T.; Ribeiro, M. J.
- CS Departamento de Fisica, IMAT (nucleo IFIMUP), CFUP, Faculdade de Ciencias da Universidade do Porto, Oporto, 4150, Port.
- SO Liquid Crystals (1998), 25(3), 375-385
CODEN: LICRE6; ISSN: 0267-8292
- PB Taylor & Francis Ltd.
- DT Journal
- LA English
- CC 75-11 (Crystallography and Liquid Crystals)
Section cross-reference(s): 73, 76
- AB Two compds. with very similar chemical formulas but different phase sequences F3H6 and F4H6, where $F_nH_m = C_nF_{2n+1}-C_mH_{2m}O-C_6H_4-COO-C_6H_4-COO-C_6H_4-COOCH(Me)-C_6H_{13}$, were studied by dielec., optical and TSM (temperature scan method) measurements, and by optical and polarization hysteresis loops. The light diffraction technique was used to measure the helical pitch (p), which is nearly temperature independent. Six relaxation modes were identified. The polarization and tilt angle results are discussed using a simple phenomenol. model and fitted to the equation $P_0/\theta_0 \approx (1/\epsilon\epsilon_0C - (\Omega/C)\theta_0^2) - 1$. The parameters C and Ω were determined from the fitting.
- ST fluorinated ferroelec antiferroelec liq crystal dielec; polarization spontaneous fluorinated ferroelec antiferroelec mesophase; helical pitch fluorinated ferroelec antiferroelec mesophase; phase sequence fluorinated ferroelec antiferroelec mesophase; relaxation frequency fluorinated ferroelec antiferroelec mesophase
- IT Liquid crystals
(antiferroelec.; dielec., optical and temperature scan method measurements on semi-perfluoro)
- IT Liquid crystals
(ferroelec.; dielec., optical and temperature scan method measurements on semi-perfluoro)
- IT Antiferroelectric materials
Ferroelectric materials
(liquid-crystal; dielec., optical and temperature scan method measurements on semi-perfluoro)
- IT Dielectric constant
Dielectric relaxation
Electrooptical effect
(of semi-perfluoro ferro- and antiferroelec. liquid crystals)
- IT Ferroelectricity

(spontaneous polarization of semi-perfluoro ferro- and antiferroelec.
liquid crystals)

IT 212779-66-3

RL: PRP (Properties)

(dielec., optical and temperature scan method measurements on semi-perfluoro
ferro- and antiferroelec. liquid crystals)

IT 212779-64-1

RL: PRP (Properties)

(dielec., optical and temperature scan method measurements on semi-perfluoro
ferroelec. liquid crystals)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

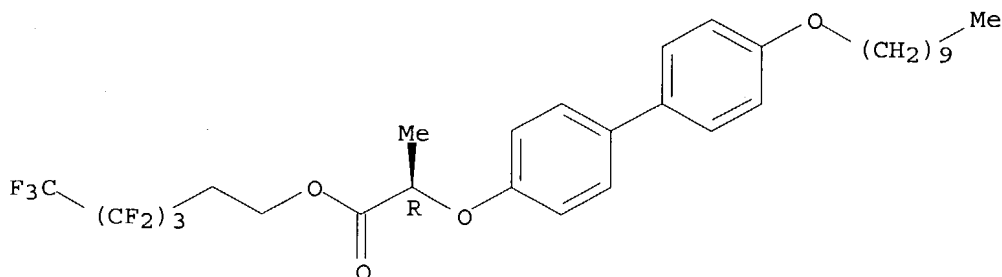
- (1) Carlsson, T; Phys Rev A 1990, V42, P877 CAPLUS
- (2) Carvalho, P; Liq Cryst 1996, V21, P115 CAPLUS
- (3) Carvalho, P; Liq Cryst 1996, V21, P511
- (4) Destrade, C; Ferroelectrics 1996, V177, P161 CAPLUS
- (5) Faye, V; Liq Cryst 1995, V19, P47 CAPLUS
- (6) Fukuda, A; J Mater Chem 1994, V4, P997 CAPLUS
- (7) Fukui, M; Jpn J appl Phys 1990, V29, P329
- (8) Goodby, J; Ferroelectric Liquid Crystals-Principles Properties and
Applications, Vol 7, Ferroelectricity and Related Phenomena 1991
- (9) Levstik, A; Phys Rev A 1987, V35, P3527 CAPLUS
- (10) Lines, M; Principles and Applications of Ferroelectrics and Related
Materials 1977
- (11) Nguyen, H; To be published
- (12) Novotna, V; Liq Cryst 1997, V23, P511 CAPLUS
- (13) Uehara, H; Jpn J appl Phys 1995, V34, P5424 CAPLUS

RN 225942-19-8 REGISTRY
 ED Entered STN: 25 Jun 1999
 CN Propanoic acid, 2-[[4'-(decyloxy)[1,1'-biphenyl]-4-yl]oxy]-,
 3,3,4,4,5,5,6,6,6-nonafluorohexyl ester, (2R)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H37 F9 O4
 CI COM
 SR CA

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	557.8+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	83.97+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.4+/-45.0 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	20		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	pH 8	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	11.60	pH 1	(1) ACD
logD (LOGD)	11.60	pH 4	(1) ACD
logD (LOGD)	11.60	pH 7	(1) ACD
logD (LOGD)	11.60	pH 8	(1) ACD
logD (LOGD)	11.60	pH 10	(1) ACD
logP (LOGP)	11.598+/-0.889		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	644.61		(1) ACD
Vapor Pressure (VP)	1.78E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

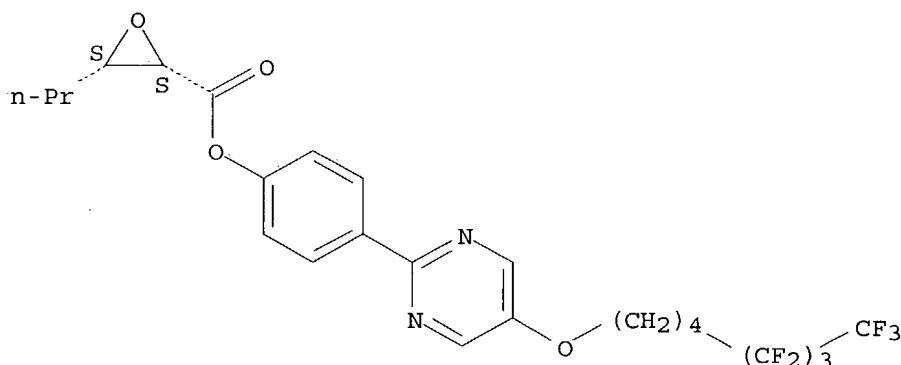
(1/3/01)
12/15/2000

RN 479201-31-5 REGISTRY
 ED Entered STN: 16 Jan 2003
 CN Oxiranecarboxylic acid, 3-propyl-, 4-[5-[(5,5,6,6,7,7,8,8,8-nonafluorooctyl)oxy]-2-pyrimidinyl]phenyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C24 H23 F9 N2 O4
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C2O	OC2	3	C2O	1.30.1	1
C6	C6	6	C6	46.150.18	1
C4N2	NCNC3	6	C4N2	46.195.39	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	4225	pH 1	(1) ACD
Bioconc. Factor (BCF)	8389	pH 4	(1) ACD
Bioconc. Factor (BCF)	8397	pH 7	(1) ACD
Bioconc. Factor (BCF)	8397	pH 8	(1) ACD
Bioconc. Factor (BCF)	8397	pH 10	(1) ACD
Boiling Point (BP)	497.0+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	76.49+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	254.4+/-51.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	14		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	11270	pH 1	(1) ACD
Koc (KOC)	22376	pH 4	(1) ACD
Koc (KOC)	22398	pH 7	(1) ACD
Koc (KOC)	22398	pH 8	(1) ACD
Koc (KOC)	22398	pH 10	(1) ACD

logD (LOGD)	5.17	pH 1	(1) ACD
logD (LOGD)	5.47	pH 4	(1) ACD
logD (LOGD)	5.47	pH 7	(1) ACD
logD (LOGD)	5.47	pH 8	(1) ACD
logD (LOGD)	5.47	pH 10	(1) ACD
logP (LOGP)	5.467+/-1.234		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	574.44		(1) ACD
pKa (PKA)	0.99+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	5.13E-10 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:64125 CA

TI Liquid crystalline materials containing perfluoroalkyl and alkenyl tail groups

IN Gough, Neil; Vohra, Rohini; Wand, Michael; More, Kundalika; Thurmes, William N.

PA USA

SO U.S. Pat. Appl. Publ., 46 pp.

CODEN: USXXCO

DT Patent

LA English

IC ICM C09K019-34

ICS C09K019-32; C09K019-30; C09K019-20; C09K019-12; C07D239-02

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CC 75-11 (Crystallography and Liquid Crystals)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002195585	A1	20021226	US 2001-754034	20010103
PRAI	US 2000-255984P		20001215		

AB This invention describes compds. that are useful as components in liquid crystal compns., particularly in ferroelec. liquid crystal compns. Compds. of the invention are rod-like mols. with a mesogenic (generally linear) core to which an alkene tail and an alkyl or alkoxy tail with a perfluoroalkyl terminal portion are bonded. Compds. of the invention can contain a variety of 1, 2 or 3 ring cores, wherein the rings maybe aromatic or alicyclic. Alkenes of the invention are useful as components to improve LC properties of mixts., for example, to lower m.p. or to lower f.p., of LC compns.

ST ferroelec liq crystal perfluoroalkyl alkenyl tail group

IT Liquid crystals

(ferroelec.; liquid crystalline materials containing perfluoroalkyl and alkenyl tail groups)

IT Ferroelectric materials

(liquid-crystal; liquid crystalline materials containing perfluoroalkyl and alkenyl tail groups)

IT Liquid crystals

(nematic; liquid crystalline materials containing perfluoroalkyl and alkenyl tail

groups)
IT Liquid crystals
(smectic; liquid crystalline materials containing perfluoroalkyl and
alkenyl tail
groups)
IT 479201-26-8P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material
use); PREP (Preparation); USES (Uses)
(liquid crystalline materials containing perfluoroalkyl and alkenyl tail
groups)
IT 57202-38-7 57202-39-8 57202-48-9 57202-54-7 57202-58-1
120091-49-8 121083-93-0 121218-85-7 121218-90-4 121235-87-8
126162-76-3 126163-69-7 155468-60-3 308107-81-5 402860-34-8
439866-35-0 460359-38-0 460359-39-1 460359-40-4 460359-42-6
460359-43-7 460359-44-8 460359-45-9 460359-51-7 479201-27-9
479201-28-0 479201-29-1 479201-30-4 479201-31-5 479201-32-6
479201-33-7 479201-34-8 479201-35-9 479201-36-0 479201-37-1
479201-38-2
RL: TEM (Technical or engineered material use); USES (Uses)
(liquid crystalline materials containing perfluoroalkyl and alkenyl tail
groups)
IT 2108-05-6, trans-3-Hepten-1-ol 2695-48-9, 8-Bromo-1-octene 20125-84-2
56578-18-8, trans-5-Decen-1-ol 64275-73-6 460359-29-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of liquid crystalline materials containing perfluoroalkyl and
alkenyl
tail groups)
IT 479201-23-5P 479201-24-6P 479201-25-7P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material
use); PREP (Preparation); USES (Uses)
(synthesis of liquid crystalline materials containing perfluoroalkyl and
alkenyl
tail groups)